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More Space-Group Corrections: From Triclinic to Centred Monoclinic and to Rhombohedral; Also From *P*1 to *P*-1 and From *Cc* to *C*2/*c*

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Material for Deposit.

More Space Group Corrections: from Triclinic to Centered Monoclinic, and to Rhombohedral; also from $P1$ to $P\bar{1}$, and from Cc to $C2/c$

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Abstract

We present fourteen examples of crystal structures that were originally described as triclinic but are properly described as either *C*-centered monoclinic (ten examples) or rhombohedral (four examples). There is also one example each of changes from $P1$ to $P\bar{1}$ and from Cc to $C2/c$.

Table 1. YAFZAG—revised coordinates in space group $C2/c$; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD (slightly modified from the original paper); atoms whose coordinates were averaged (after transformation) are bracketed here, and elsewhere in these tables.

Pairs of related atoms TTF Molecule	x	y	z
S(1,3)	0.0305[0]	0.1775[5]	-0.0650[1]
S(2,4)	-0.0840[0]	0.1610[1]	-0.1182[1]
C(1,4)	-0.0109[2]	0.0719[3]	-0.0387[2]
C(2,5)	-0.0264[2]	0.3201[21]	-0.1676[5]
C(3,6)	-0.0782[1]	0.3100[60]	-0.1907[8]
DMeT-DCNQI Molecule			
S(5,6)	-0.2657[0]	0.5170[3]	-0.1622[2]
C(7,12)	-0.2000[6]	0.6583[45]	-0.1379[11]
C(8,13)	-0.2538[4]	0.6497[16]	-0.0705[4]
C(9,14)	-0.2085[8]	0.8537[1]	-0.0056[0]
C(10,15)	-0.2978[7]	0.5449[7]	-0.0667[8]
C(11,16)	-0.3818[1]	0.2385[8]	-0.1305[1]
N(1, 3)	-0.3408[1]	0.3468[19]	-0.1317[1]
N(2, 4)	-0.4188[8]	0.1274[25]	-0.1360[6]

Table 2. BAHZEP10—revised coordinates in space group $C2/m$; Δ(fit) values are given in square brackets. The atom numbering is that used in the original paper and in the CSD.

Related atoms	x	y	z
Br	-0.3414	0.5000[1]	0.4840
C(1)	-0.1992	0.5000[4]	0.3826
C(2,3)	-0.2237[1]	0.3787[9]	0.2246[5]
C(4)	-0.0236	0.5000[6]	0.5926
C(5,6)	-0.0683[1]	0.3784[4]	0.2394[7]
H(21,31)	-0.326[6]	0.384[1]	0.071[6]
H(22,32)	-0.246[4]	0.307[6]	0.294[18]
H(51,61)	-0.083[5]	0.388[7]	0.078[2]
H(52,62)	-0.002[0]	0.299[4]	0.297[6]

Table 3. KORZIA—revised coordinates in space group C2/c; Δ(fit) values are given in square brackets. The atom numbering given here is that used in the CSD, and differs from that of the original paper.

Pairs of related atoms	x	y	z
Cl(1,2)	0.3880[5]]	0.5443[13	0.2272[4]
C(1,8)	0.3045[2]	0.4492[26]	0.1629[7]
C(2,9)	0.2523[7]	0.2642[40]	0.1730[26]
C(3,10)	0.1877[6]	0.1966[52]	0.1216[11]
C(4,11)	0.1743[3]	0.3282[10]	0.0640[24]
C(5,12)	0.2257[39]	0.5141[104]	0.0552[13]
C(6,13)	0.2924[33]	0.5762[69]	0.1062[10]
C(7,14)	-0.0020[53]	0.4625[40]	-0.1431[3]
N(1,4)	0.1050[4]	0.2580[31]	0.0126[22]
N(2,5)	0.0867[19]	0.3959[12]	-0.0406[18]
N(3,6)	0.0246[29]	0.3192[49]	-0.0818[1]
O(1,2)	-0.0147[18]	0.1132[9]	-0.0736[10]
H(1,4)	0.0325[57]	0.6454[287]	-0.1476[22]
H(2,6)	-0.0624[19]	0.5185[563]	-0.1528[23]
H(3,5)	0.0037[135]	0.3057[88]	-0.1774[4]
H(7,12)	0.0796[132]	0.1766[514]	0.0273[19]
H(8,13)	0.2524[32]	0.2092[716]	0.2143[14]
H(9,14)	0.1390[226]	0.1042[96]	0.1300[55]
H(10,15)	0.2368[97]	0.5134[236]	0.0122[18]
H(11,16)	0.3235[25]	0.7002[1067]	0.0990[50]

Some of the original (triclinic) coordinates of the hydrogen atoms may have been misprinted, as several of the C(-H and N-H bond lengths are unreasonable.

Table 4. FAKROY—revised coordinates in space group *Cc*; Δ(fit) values are given in square brackets. The atom numbering is that used in the original paper and in the CSD.

Pairs of related atoms	x	y	z
C(1, 9)	-0.2643[20]	0.2342[15]	0.2568[22]
C(2, 10)	-0.2873[20]	0.3706[7]	0.3364[99]
C(3, 11)	-0.3344[4]	0.3557[24]	0.3242[90]
C(4, 12)	-0.3611[6]	0.2200[40]	0.2324[45]
C(5, 13)	-0.3387[4]	0.0876[12]	0.1494[35]
C(6, 14)	-0.2911[5]	0.0891[16]	0.1654[34]
C(7, 15)	-0.2156[1]	0.2490[5]	0.2671[33]
C(8, 16)	-0.1993[7]	0.2136[6]	0.0876[10]
N(1, 2)	-0.1828[4]	0.2932[22]	0.4114[10]
O(1, 2)	-0.1966[3]	0.3132[22]	0.5776[16]
C(17, 25)	-0.0273[2]	0.7474[22]	0.4877[10]
C(18, 26)	-0.0165[0]	0.6484[22]	0.6622[8]
C(19, 27)	0.0277[5]	0.6451[8]	0.7684[34]
C(20, 28)	0.0627[0]	0.7419[8]	0.7120[102]
C(21, 29)	0.0530[12]	0.8302[16]	0.5508[24]
C(22, 30)	0.0078[2]	0.8427[33]	0.4334[50]
C(23, 31)	-0.0764[7]	0.7605[14]	0.3726[63]
C(24, 32)	-0.0904[2]	0.9375[9]	0.2533[64]

N(3, 4)	-0.1094[2]	0.6425[11]	0.3448[12]
O(3, 4)	-0.0960[7]	0.4658[6]	0.4368[9]

Table 5. WEGFIX — revised coordinates in space group C2; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD.

Pairs of related atoms	x	y	z
V(1,2)	0.14310[0]	-0.09999[1]	0.19014[10]
O(1)	0.0000[1]	-0.0711	0.0000[0]
O(2,6)	0.0788[0]	-0.2115[0]	0.2404[1]
O(3,7)	0.0876[0]	-0.2765[0]	0.4395[0]
O(4,8)	0.3976[0]	-0.2542[0]	0.2932[0]
O(5,9)	0.4605[1]	-0.1869[1]	0.1732[4]
N(1,7)	0.3002[2]	-0.1545[0]	0.4314[0]
N(2,8)	0.1260[1]	-0.0094[2]	0.3329[2]
N(3,9)	0.0625[0]	0.1105[1]	0.3932[2]
N(4,10)	0.1711[0]	-0.2045[0]	0.0663[0]
N(5,11)	0.2529[0]	-0.0026[0]	0.1920[3]
N(6,12)	0.3872[1]	0.1080[1]	0.2687[0]
C(1,13)	0.1307[1]	-0.2300[0]	0.3900[0]
C(2,14)	0.2560[1]	-0.1864[1]	0.5160[2]
C(3,15)	0.2516[1]	-0.1006[1]	0.6035[0]
C(4,16)	0.1723[2]	-0.0203[0]	0.4942[0]
C(5,17)	0.0596[2]	0.0698[0]	0.2760[0]
C(6,18)	0.1340[0]	0.0544[1]	0.5326[0]
C(7,19)	0.3815[3]	-0.2100[1]	0.1792[7]
C(8,20)	0.2512[0]	-0.1860[0]	0.0282[0]

C(9,21)	0.2347[1]	-0.0840[1]	-0.0348[4]
C(10,22)	0.2846[1]	-0.0098[1]	0.0938[3]
C(11,23)	0.3161[0]	0.0692[0]	0.2956[2]
C(12,24)	0.3684[1]	0.0600[1]	0.1426[0]

Table 6. WEGTUX—revised coordinates in space group C2; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD.

Pairs of related atoms	x	y	z
W(1,18)	-0.1792[1]	0.4589[6]	-0.3635[3]
W(2,17)	-0.1103[1]	0.2698[3]	-0.3565[1]
W(3,16)	-0.0410[1]	0.4604[3]	-0.3482[1]
W(4,13)	-0.1866[0]	0.3925[1]	-0.1517[1]
W(5,12)	-0.1157[0]	0.2016[0]	-0.1434[1]
W(6,11)	0.0328[1]	0.2012[2]	-0.1287[0]
W(7,10)	0.1021[1]	0.3923[1]	-0.1211[1]
W(8,15)	0.0273[0]	0.5962[2]	-0.1283[0]
W(9,14)	-0.1124[0]	0.5965[0]	-0.1449[1]
Cl(1,2)	-0.0427[6]	0.3992[6]	-0.1391[3]
O(1,62)	-0.249[0]	0.501[0]	-0.456[0]
O(2,61)	-0.179[3]	0.353[1]	-0.412[1]
O(3,59)	-0.126[3]	0.493[3]	-0.404[4]
O(4,57)	-0.077[0]	0.400[1]	-0.250[3]
O(5,49)	-0.197[1]	0.413[2]	-0.276[3]
O(6,53)	-0.145[1]	0.551[1]	-0.270[0]
O(7,60)	-0.136[3]	0.196[0]	-0.446[0]
O(8,46)	-0.132[1]	0.236[1]	-0.269[4]
O(9,58)	-0.070[1]	0.350[1]	-0.397[1]
O(10,42)	-0.031[1]	0.234[0]	-0.261[0]

O(11,56)	-0.023[3]	0.503[2]	-0.430[5]
O(12,55)	-0.018[2]	0.552[0]	-0.258[1]
O(13,39)	0.035[1]	0.412[2]	-0.252[1]
O(14,47)	-0.260[3]	0.410[1]	-0.182[6]
O(15,44)	-0.182[1]	0.275[2]	-0.166[1]
O(16,48)	-0.155[2]	0.509[1]	-0.128[3]
O(17,45)	-0.081[2]	0.355[1]	-0.112[1]
O(18,28)	-0.148[1]	0.381[1]	-0.016[2]
O(19,43)	-0.147[5]	0.107[1]	-0.167[6]
O(20,41)	-0.035[1]	0.185[1]	-0.114[0]
O(21,25)	-0.084[0]	0.211[1]	-0.008[0]
O(22,40)	0.052[2]	0.105[2]	-0.149[2]
O(23,37)	0.089[2]	0.274[0]	-0.138[5]
O(24,38)	0.014[0]	0.356[1]	-0.104[0]
O(26,35)	0.162[2]	0.410[2]	-0.136[4]
O(27,36)	0.083[1]	0.507[0]	-0.102[5]
O(29,54)	0.062[1]	0.683[0]	-0.144[2]
O(30,52)	-0.045[2]	0.647[1]	-0.148[2]
O(31,51)	-0.034[2]	0.488[0]	-0.110[2]
O(32,34)	0.063[1]	0.611[0]	0.006[1]
O(33,50)	-0.158[0]	0.684[0]	-0.170[1]
N(1)	0[5]	-0.0100*	0[3]
N(2,3)	-0.340[1]	0.138[0]	-0.304[3]
C(1,5)	0.046[4]	-0.158[0]	0.000[7]
C(2,6)	0.100[4]	-0.098[2]	0.002[15]
C(3,7)	0.140[2]	-0.151[7]	0.002[0]
C(4,8)	0.187[7]	-0.104[0]	-0.018[17]

C(9,13)	0.032[0]	-0.047[0]	0.086[2]
C(10,14)	0.064[4]	-0.084[1]	0.190[0]
C(11,15)	0.098[24]	-0.020[11]	0.284[15]
C(12,16)	0.109[9]	-0.015[2]	0.355[2]
C(17,33)	-0.355[5]	0.046[1]	-0.326[2]
C(18,34)	-0.294[0]	-0.009[1]	-0.308[2]
C(19,35)	-0.325[9]	-0.098[0]	-0.342[5]
C(20,36)	-0.280[2]	-0.143[4]	-0.326[13]
C(21,37)	-0.313[2]	0.186[0]	-0.349[3]
C(22,38)	-0.358[1]	0.184[1]	-0.456[3]
C(23,39)	-0.317[2]	0.224[5]	-0.498[5]
C(24,40)	-0.357[4]	0.234[2]	-0.598[10]
C(25,45)	-0.400[0]	0.178[3]	-0.326[3]
C(26,46)	-0.397[7]	0.270[1]	-0.312[10]
C(27,47)	-0.464[4]	0.296[10]	-0.348[5]
C(28,48)	-0.462[26]	0.380[6]	-0.338[19]
C(29,41)	-0.292[2]	0.156[1]	-0.202[1]
C(30,42)	-0.296[1]	0.126[4]	-0.116[3]
C(31,43)	-0.242[6]	0.146[6]	-0.016[3]
C(32,44)	-0.253[4]	0.107[4]	0.049[9]

*y coordinate of N(1) fixed at this (arbitary) value.

Table 7. YOVVIO—revised coordinates in space group C2; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD.

Pairs of related atoms	x	y	z
C(1,43)	0.0565[7]	0.1889[3]	0.2544[14]
C(2,44)	0.0962[11]	0.1945[5]	0.1856[16]
C(3,45)	0.1376[5]	0.1423[13]	0.1842[6]
C(4,46)	0.1883[2]	0.1319[5]	0.2803[2]
C(5,47)	0.1443[5]	0.1244[2]	0.3409[1]
C(6,48)	0.1896[15]	0.1141[4]	0.4384[21]
O(1,38)	0.2261[5]	0.0802[1]	0.2733[9]
O(2,39)	0.1032[5]	0.1730[5]	0.3378[8]
O(3,40)	0.0442[13]	0.2046[2]	0.1028[11]
O(4,41)	0.1816[1]	0.1505[2]	0.1262[1]
O(5,42)	0.2351[6]	0.1560[12]	0.4724[17]
C(7,49)	0.3041[11]	0.0781[9]	0.3130[9]
C(8,50)	0.3332[4]	0.0563[0]	0.2434[6]
C(9,51)	0.3095[6]	-0.0034[4]	0.2225[9]
C(10,52)	0.3334[7]	-0.0335[8]	0.3057[13]
C(11,53)	0.3026[11]	-0.0106[4]	0.3734[11]
C(12,54)	0.3228[6]	-0.0364[5]	0.4602[8]
O(6,43)	0.3025[9]	-0.0889[1]	0.2842[9]
O(7,44)	0.3257[6]	0.0460[5]	0.3878[1]
O(8,45)	0.3127[2]	0.0888[0]	0.1658[9]

O(9,46)	0.3425[2]	-0.0252[1]	0.1610[1]
O(10,47)	0.3974[1]	-0.0386[6]	0.5002[18]
C(13,55)	0.3524[11]	-0.1341[5]	0.3082[4]
C(14,56)	0.3385[7]	-0.1694[3]	0.2302[10]
C(15,57)	0.2604[12]	-0.1915[0]	0.2042[18]
C(16,58)	0.2492[3]	-0.2204[9]	0.2819[13]
C(17,59)	0.2711[13]	-0.1841[2]	0.3636[0]
C(18,60)	0.2716[8]	-0.2132[9]	0.4464[6]
O(11,48)	0.1712[1]	-0.2329[4]	0.2559[6]
O(12,49)	0.3412[2]	-0.1630[5]	0.3796[0]
O(13,50)	0.3508[2]	-0.1408[4]	0.1598[8]
O(14,51)	0.2465[5]	-0.2275[3]	0.1334[6]
O(15,52)	0.3254[8]	-0.2573[6]	0.4664[4]
C(19,61)	0.1522[0]	-0.2842[7]	0.2737[13]
C(20,62)	0.1009[4]	-0.3063[3]	0.1864[6]
C(21,63)	0.0305[9]	-0.2767[0]	0.1561[5]
C(22,64)	-0.0038[1]	-0.2756[0]	0.2302[14]
C(23,65)	0.0492[13]	-0.2535[8]	0.3137[2]
C(24,66)	0.0220[13]	-0.2528[13]	0.3914[21]
O(16,53)	-0.0700[4]	-0.2447[4]	0.2018[4]
O(17,54)	0.1166[8]	-0.2828[3]	0.3392[4]
O(18,55)	0.1357[7]	-0.3086[1]	0.1229[1]
O(19,56)	-0.0206[2]	-0.3028[5]	0.0782[6]
O(20,57)	0.0103[10]	-0.2979[14]	0.4089[13]
C(25,67)	-0.1357[8]	-0.2692[2]	0.2042[9]
C(26,68)	-0.1936[17]	-0.2609[4]	0.1184[13]
C(27,69)	-0.2085[4]	-0.1992[7]	0.1015[4]

C(28,70)	-0.2284[3]	-0.1756[2]	0.1776[7]
C(29,71)	-0.1710[6]	-0.1909[0]	0.2673[10]
C(30,72)	-0.1949[15]	-0.1763[12]	0.3448[6]
O(22,58)	-0.2331[4]	-0.1196[1]	0.1666[10]
O(23,59)	-0.1562[8]	-0.2463[3]	0.2736[6]
O(24,60)	-0.1713[1]	-0.2836[5]	0.0460[6]
O(25,61)	-0.2666[9]	-0.1901[3]	0.0230[3]
O(26,62)	-0.2553[0]	-0.2068[12]	0.3417[30]
C(31,73)	-0.2968[1]	-0.0926[0]	0.1732[7]
C(32,74)	-0.3258[1]	-0.0582[5]	0.0943[26]
C(33,75)	-0.2767[20]	-0.0111[5]	0.0884[17]
C(34,76)	-0.2571[8]	0.0194[2]	0.1772[11]
C(35,77)	-0.2273[25]	-0.0172[5]	0.2552[8]
C(36,78)	-0.2296[70]	0.0134[27]	0.3354[16]
O(28,64)	-0.2000[8]	0.0592[1]	0.1760[1]
O(29,65)	-0.2796[2]	-0.0608[1]	0.2500[4]
O(30,66)	-0.3450[6]	-0.0880[4]	0.0096[8]
O(31,67)	-0.3054[12]	0.0236[3]	0.0170[2]
O(32,68)	-0.1722[5]	-0.0158[0]	0.4074[11]
C(37,79)	-0.2130[13]	0.1130[10]	0.1874[20]
C(38,80)	-0.1990[2]	0.1441[4]	0.1129[9]
C(39,81)	-0.1209[4]	0.1393[1]	0.1204[0]
C(40,82)	-0.0743[2]	0.1581[7]	0.2131[11]
C(41,83)	-0.0940[3]	0.1310[8]	0.2849[1]
C(42,84)	-0.0598[0]	0.1526[2]	0.3728[4]
O(33,69)	0.0011[2]	0.1453[2]	0.2216[4]
O(34,70)	-0.1727[2]	0.1340[0]	0.2681[2]

O(35,71)	-0.2454[1]	0.1285[2]	0.0312[1]
O(36,72)	-0.1024[1]	0.1708[1]	0.0552[0]
O(37,73)	-0.0688[1]	0.2078[4]	0.3796[4]
O(74,91)	0.3574[4]	0.1978[8]	0.4381[12]
O(75,87)	0.3558[9]	0.1028[2]	-0.4171[42]
O(76,88)	0.4134[30]	-0.0614[25]	-0.3300[9]
O(77,-)	0.0000[16]	0.0483[-]	0.5000[22]
O(78,-)	0.0000[5]	0.3774[-]	0.5000[12]
O(79,89)	-0.0459[0]	0.2867[2]	-0.4223[12]
O(80,90)	0.1038[7]	0.3294[13]	0.3030[3]
O(81,92)	0.0878[[8]	0.2907[10]	0.0224[2]
O(82,93)	0.4401[19]	0.0921[8]	0.1274[85]
O(83,94)	-0.0231[2]	0.3214[15]	0.1457[32]
O(84,95)	-0.4198[10]	0.0892[3]	0.0503[1]
O(85,-)	-0.5000[15]	-0.0965[-]	0.0000[168]
O(86,96)	0.0134[9]	0.4644[59]	-0.1334[58]

Table 8. CLEOZP10—revised coordinates in space group *R*3, using hexagonal axes; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD.

Triples of related atoms	x	y	z
P(1,2,3)	-0.0478[3]	-0.1892[3]	-0.0552[4]
O(1,3,5)	-0.0518[7]	-0.2736[2]	-0.1224[18]
C(1,8,15)	-0.0316[13]	-0.2614[13]	-0.2560[15]
C(2,9,16)	-0.1023[1]	-0.2507[11]	-0.3196[18]
C(3,10,17)	-0.1025[3]	-0.1675[2]	-0.2785[9]
N(1,3,5)	-0.1096[13]	-0.1638[10]	-0.1437[16]
O(2,4,6)	0.0468[11]	-0.1183[11]	-0.0296[9]
N(2,4,6)	-0.1041[6]	-0.2281[3]	0.0759[3]
C(4,11,18)	-0.2017[9]	-0.2908[14]	0.0751[10]
C(5,12,19)	-0.2504[20]	-0.2404[11]	0.1097[5]
C(6,13,20)	-0.0488[2]	-0.2211[10]	0.1974[21]
C(7,14,21)	-0.0399[10]	-0.1433[22]	0.2484[15]
Cl(1,3,5)	-0.3707[2]	-0.3157[2]	0.1081[5]
Cl(2,4,6)	0.0345[1]	-0.1272[1]	0.3920[4]

Table 9. BALFEZ—revised coordinates in space group $R\bar{3}$, using hexagonal axes; Δ(fit) values are given in square brackets. The atom numbering is that used in the CSD.

Triples of related atoms	x	y	z
Molecule 1, centred at 000; site symmetry $\bar{3}$			
Cluster			
Cu(1,2,3)	-0.01231[2]	-0.04441[2]	0.0937[1]
S(1,2,3)	-0.04670[12]	-0.03340[7]	0.1853[3]
N(1,2,3)	-0.0848[2]	-0.0583[2]	-0.0038[7]
C(1,2,3)	-0.0829[0]	-0.0589[2]	0.1164[12]
Morpholino group			
N(19,20,21)	-0.1057[2]	-0.0792[1]	0.1981[3]
C(37,41,45)	-0.1326[4]	-0.1089[3]	0.1624[17]
C(38,42,46)	-0.1364[7]	-0.1341[4]	0.2487[15]
O(7,8,9)	-0.1389[2]	-0.1269[2]	0.3727[8]
C(39,43,[47]) *	-0.1117[1]	-0.0991[1]	0.4119[28]
C(40,44,48)	-0.1064[2]	-0.0731[3]	0.3322[25]
Molecule 2, site symmetry $\bar{1}$, centered at 1/2,1/2,0			
Cluster			
Cu(4,7,11)	0.51577[12]	0.48740[9]	-0.1573[1]
Cu(5,9,10)	0.45362[4]	0.46214[8]	0.0038[2]
Cu(6,8,12)	0.49226[4]	0.53278[2]	-0.1046[2]

S(4,7,11)	0.44203[12]	0.49760[12]	-0.0720[1]
S(5,9,10)	0.51442[14]	0.52428[11]	-0.2759[1]
S(6,8,12)	0.47150[7]	0.44247[9]	-0.1445[3]
C(4,7,11)	0.4317[2]	0.5121[2]	0.0626[3]
C(5,9,10)	0.5527[2]	0.5546[3]	-0.2695[7]
C(6,8,12)	0.4787[2]	0.4155[1]	-0.0644[2]
N(4,7,11)	0.4432[2]	0.5122[2]	0.1707[1]
N(5,9,10)	0.5675[3]	0.5622[4]	-0.1601[2]
N(6,8,12)	0.4902[5]	0.4220[3]	0.0518[8]

Morpholino group 1

N(14,16,22)	0.4101[2]	0.5212[1]	0.0376[8]
C(17,25,52)	0.3958[2]	0.5193[5]	-0.0906[8]
C(18,26,51)	0.3714[5]	0.5249[2]	-0.0902[6]
O(2,4,10)	0.3749[2]	0.5501[3]	-0.0220[2]
C(19,27,50)	0.3867[2]	0.5517[2]	0.1045[2]
C(20,28,49)	0.4136[2]	0.5492[4]	0.1090[2]

Morpholino group 2

N(13,17,24)	0.5653[3]	0.5695[2]	-0.3834[5]
C(13,29,57)	0.5526[3]	0.5540[4]	-0.5052[7]
C(14,30,58)	0.5797[2]	0.5663[1]	-0.5994[5]
O(1,5,12)	0.5947[9]	0.5991[7]	-0.6126[9]
C(15,31,59)	0.6071[2]	0.6142[3]	-0.4949[11]
C(16,32,[60])	0.5812[4]	0.6032[0]	-0.3959[2]

**

Morpholino group 3

N(15,18,23)	0.4729[4]	0.3898[2]	-0.1299[5]
C(21,33,53)	0.4554[7]	0.3804[2]	-0.2499[6]
C(22,34,52)	0.4758[5]	0.3841[3]	-0.3507[11]
O(3,6,11)	0.4907[2]	0.3649[2]	-0.3343[4]
C(23,35,55)	0.5082[4]	0.3755[4]	-0.2181[19]
C(24,36,56)	0.4894[3]	0.3723[6]	-0.1085[13]

* Coordinates of C(47) are incorrect so it was not included in the averaging.

** Coordinates of C(60) were not given so it could not be included in the averaging.

Table 10. ENICCU—revised coordinates in space group $R\bar{3}$, using hexagonal axes (obverse setting); Δ(fit) values are given in square brackets. The same atom numbering is used in the CSD and the original paper.

Triples of related atoms	x	y	z
Cu(1,2,3)	0.0	0.5	0.5
Cl(1,2,3)	-0.0672[2]	0.4476[4]	0.6666[4]
O(1,2,3)	-0.1954[5]	0.5694[5]	0.3418[11]
N(1,3,5)	-0.0263[12]	0.5683[7]	0.5023[13]
N(2,4,6)	-0.2229[5]	0.5409[5]	0.5499[5]
C(1,11,21)	0.0154[7]	0.6299[5]	0.5189[15]
C(2,12,22)	-0.0004[7]	0.6778[0]	0.5171[13]
C(3,13,23)	-0.0683[13]	0.6573[6]	0.4993[15]
C(4,14,24)	-0.1099[4]	0.5932[5]	0.4839[4]
C(5,15,25)	-0.0900[3]	0.5483[9]	0.4870[12]
C(6,16,26)	-0.1809[8]	0.5662[7]	0.4516[13]
C(7,17,27)	-0.2044[2]	0.5454[10]	0.6851[13]
C(8,18,28)	-0.2083[17]	0.4863[15]	0.7373[23]
C(9,19,29)	-0.2946[2]	0.5102[10]	0.5189[16]
C(10,20,30)	-0.3254[13]	0.4371[20]	0.4894[39]

Table 11. x,y,z Coordinates averaged for the centrosymmetric $C_{38}H_{30}N_2O_{10}Cu_2$ molecule in the reduced $P\bar{1}$ unit cell (see text for details of missing atoms); Δ(fit) values are given in square brackets. The atom numbering is that of Yang *et al.*, 1997.

Paired atoms	x	y	z
Cu(1, 2)	0.621[2]	0.557[1]	0.467[1]
O(1, 3)	0.495[3]	0.741[3]	0.340[1]
O(2, 4)	0.709[2]	0.357[1]	0.606[3]
O(5, 7)	0.676[3]	0.494[5]	0.317[5]
O(6, 8)	0.527[1]	0.606[4]	0.626[0]
O(9, 10)	0.823[3]	0.643[2]	0.408[2]
N(1, 2)	0.830[4]	0.724[3]	0.466[1]
C(1, 3)	0.364[4]	0.748[1]	0.327[1]
C(2, 4)	0.405[3]	0.569[1]	0.702[2]

Table 12. FAKRIS01—x,y,z coordinates averaged for molecules 1 and 3, and for molecules 2 and 4, in space group *C2/c*; Δ(fit) values are given in square brackets. The atom numbering is that of the CSD.

Pairs of related atoms	mean $x_{1,3}$	mean $y_{1,3}$	mean $z_{1,3}$
C(1,17)	0.0662[33]	-0.6003[51]	-0.0239[58]
C(2,18)	0.0862[37]	-0.4670[351]	-0.0702[2]
C(3,19)	0.0820[34]	-0.5109[164]	-0.1487[72]
C(4,20)	0.0554[14]	-0.6855[132]	-0.1810[60]
C(5,21)	0.0350[35]	-0.8157[41]	-0.1360[13]
C(6,22)	0.0410[26]	-0.7794[76]	-0.0568[37]
C(7,23)	0.0717[24]	-0.5607[85]	0.0600[54]
C(8,24)	0.0504[6]	-0.7214[110]	0.1106[31]
N(1,3)	0.0958[6]	-0.3802[8]	0.0847[55]
O(1,3)	0.0996[5]	-0.3530[19]	0.1641[35]
	mean $x_{2,4}$	mean $y_{2,4}$	mean $z_{2,4}$
C(9,25)	0.1860[10]	0.2043[151]	0.2652[55]
C(10,26)	0.1685[10]	0.0307[14]	0.3083[18]
C(11,27)	0.1740[13]	0.0387[71]	0.3868[43]
C(12,28)	0.1994[13]	0.2204[60]	0.4260[15]
C(13,29)	0.2174[6]	0.3895[41]	0.3854[12]
C(14,30)	0.2107[10]	0.3836[180]	0.3040[33]
C(15,31)	0.1800[22]	0.1990[38]	0.1808[23]

C(16,32)	0.2000[4]	0.3829[40]	0.1350[55]
N(2,4)	0.1561[7]	0.0232[100]	0.1500[37]
O(2,4)	0.1512[28]	0.0200[66]	0.0696[61]